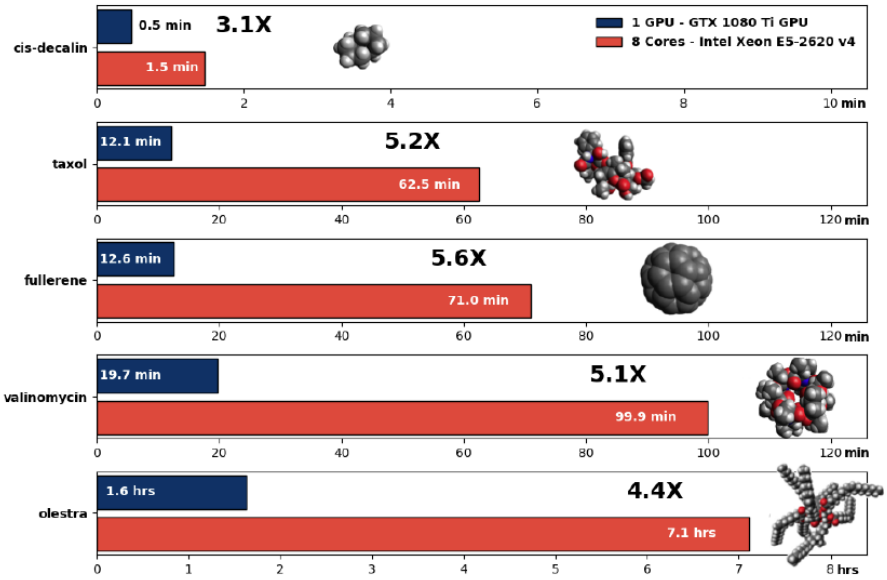
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

BrianQC GPU Acceleration Module



Wall time of a Hartree-Fock energy evaluation in the cc-pVTZ basis set

- Available as an add-on for Q-Chem 5.0 or later;
- Optimized for simulating large molecules;
- Tested on systems up to 20,000 basis functions;
- Supports basis sets with function of up to g angular momentum;
- Full support for all NVIDIA GPU architectures (Kepler, Maxwell, Pascal, Volta);
- Effectively utilizes low-cost gaming GPUs;
- Multi-GPU and supercomputer support;
- Mixed-precision operation delivers results with double-precision accuracy;
- Accelerates J and K matrix and first derivative calculations;
- GPU-accelerated XC matrix evaluation;
- Up to 6x speedup for SCF.

Request a free trial at www.q-chem.com